Acetic acid, (hexyloxy)-57931-25-6 | DTXSID9069211

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 281 °C

Global applicability domain: Inside

Local applicability domain index: 6.52e-01

Confidence level: 5.82e-01

Nearest Neighbors from the Training Set

Image not found

9-Cycloheptadecen-1-one

Measured: 343 Predicted: 330 Image not found

Nonanoic acid Measured: 255 Predicted: 260 Image not found

Cyclohexanepropionic acid

Measured: 277 Predicted: 279

Image not found

Octanoic acid Measured: 239 Predicted: 235 Image not found

Decanoic acid Measured: 269 Predicted: 277